U.S. High Production Volume (HPV) Chemical Challenge Program

PROPOSED TEST PLAN FOR ZINC NAPHTHENATE

CASRN 12001-85-3

Prepared by

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on behalf of

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Sponsoring Members of the

The Metal Carboxylates Coalition

A SOCMA Affiliated Consortium

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Summary

Zn naphthenate is one of 19 metal carboxylate compounds being sponsored by the Metal Carboxylates Coalition a SOCMA affiliated consortium. HPV endpoints for Zn naphthenate are filled using a comprehensive existing data set for the metal salt, which is a registered pesticide under the Federal Insecticide Fungicide and Rodenticide Act (FIFRA). In addition, the metal salt data is supported by data for the dissociations products (i.e., the metal and the carboxylic acid). Selected testing of the parent molecules has been proposed to fill HPV endpoints not filled by the existing FIFRA dossier. Because metal carboxylates such as Zn naphthenate readily dissociate into the corresponding metal and carboxylic acid, Robust summaries are provided for the parent molecules (Zn naphthenate), and the metal (Zn) and the acid (naphthenic acid). The summary of existing data and proposed testing is presented in the Test Plan Matrix (Table 1)

Use Patterns for Metal Carboxylates

The metal carboxylates function to deliver a metal ion into chemical reactions. The carboxylic acids (acids) are designed for use in different products or chemical reactions. Zinc carboxylate compounds are used as catalysts in paints and coatings; and in polyurethanes. They are used as heat stabilizers for PVC and as a heat and/or friction modifiers for lubricants and greases. Zinc carboxylate compounds can also be used as wetting agent for pigments in organic systems.

Characteristics of Zn Naphthenate

The metal carboxylate salts are designed to add metals to chemical reactions; therefore, they are designed to readily dissociate into the free metal and free acid. The dissociation constant is important because it determines the proportion of acid or metal that is dissociated at a given pH. The free acid and corresponding free metal are often much different than the salt (ion pair) moiety in characteristics such as solubility, adsorption, and toxicity. The proportion of dissociation influences the behavior of the substance in the environment and bioavailability of the acid and metal constituents of metal carboxylate salts. The dissociation constant (pKa) for Zn naphthenate is 7.31.

Zinc naphthenate may be a viscous liquid containing 8-10% zinc or a solid containing 16% zinc (EPA 1992). The molecular weight ranges from approximately 381 to 813. The molecular formula is described by:

$$Zn(MRCO_2)(NRCO_2)$$

Where, R = alkyl group with a chain length of 0 to 10 carbon atoms. M & N are typically one or two fused rings (usually cyclopentane, but occasionally cyclohexane and heptane rings) that may contain one or more alkyl substitutions. The total number of carbon atoms in M or N ranges from about 9 to 25. In some cases, no fused ring is present and M or N may be straight-chain or multiple branched carbon/hydrogen/oxygen molecules

Dissociation Products:

This submission relies primarily on the existing FIFRA data set for Zn naphthenate. However, because the dissociation products (metal and acid) are important to understanding the environmental fate and effects of the parent metal carboxylate robust summaries for the dissociation products are provided as part of this submission.

Test Plan Summary and Conclusions:

The test plan and summary conclusions made by the Coalition are summarized in the Test Plan Matrix (Table 1). The Coalition has proposed the following:

Physicochemical Properties

Adequate data is available for the physicochemical properties (Test Plan Matrix, Table 1). This GLP data was generated as part of a FIFRA submission under 40 CFR 158. No additional testing is recommended.

Environmental Fate Parameters:

Biodegradation: An evaluation of the biodegradation of Zn naphthenate is unnecessary. The parent, metal salt, dissociates into Zn which does not biodegrade and naphthenic acid which is known to biodegrade (Hemen et al. 1994). Therefore, the Coalition will depend on the data for the naphthenic acid to fill this data element.

Photodegradation: In solution Zn naphthenate will dissociate. Zn will not photodegrade. Naphthenic acid is a complex distillate fraction for which photodegradation cannot be estimated or accurately measured. This data element will not be filled. No testing is recommended.

Transport: Fugacity models rely upon a substance being pure and non-ionized and are inappropriate for a metal carboxylate such as Zn naphthenate which

dissociates into ionized moieties. In addition, naphthenate is not a pure chemical, but a complex petroleum distillate fraction. Fugacity modeling is considered inappropriate for Zn naphthenate. No testing is recommended.

Ecotoxicity:

Adequate ecotoxicity data are available for fish and invertebrate species for Zn naphthenate; however, data for aquatic plant (green algae) toxicity was needed. No data for the acid (naphthenic acid) was available and data for Zn indicates algae may be more sensitive to this metal than the animal species. Testing has been conducted to address this endpoint (as reflected in Test Plan Matrix Table 1). See Robust Summaries for the specific data.

Human Health Effects:

Because Zn naphthenate is a FIFRA registered product a complete set of GLP studies reviewed by the EPA are available, including for acute mammalian (oral, inhalation, dermal, skin irritation, eye irritation) toxicity studies, genotoxicity (gene mutation and chromosomal aberration) and higher tiered mammalian studies (i.e., repeated dose, reproduction, and developmental toxicity) are available for Zn naphthenate (See Robust Summaries for more detail); therefore, no additional studies are proposed for this chemical (Test Plan Matrix, Table 1).

Summary of Test Plan

In summary, the only data element that needed to be filled was the algal toxicity for which a study has been completed. This data has been incorporated into the Test Plan and Robust Summaries (Table 1). All data gaps are filled and no additional testing is required.

Table 1 Test Plan Matrix: Zn Naphthenate

	Information available	GLP Study	Information for Dissociation Products	Acceptable	Testing recommended
PHYSICOCHEMICAL PROPERTIES					
Melting Point	Y	Y	N	Y	N
Boiling Point	Y	Y	N	Y	N
Vapor pressure	Y	U[a]	N	Y	N
Partition Coefficient	Y	Y	N	Y	N
Water Solubility	Y	Y	Y	Y	N
ENVIRONMENTAL FATE PARAMETERS					
Photodegradation	N	--[b]	--	--	N
Dissociation in water	Y	Y	--	Y	N
Transport	--	--	--	--	N
Biodegradation	N	--	Y	Y	N
ECOTOXICITY					
Fish toxicity (96-h)	Y	Y	Y	Y	N
Invertebrate toxicity (48-h	Y	Y	Y	Y	N
Algae toxicity (72-h)	***Y[c]***	***Y[c]***	Y	***Y[c]***	***N[c]***
TOXICITY					
Acute	Y	N	Y	Y	N
Repeated dose	Y	Y	N	Y	N
Genetic Toxicology – mutation assay	Y	Y	Y	Y	N
Genetic Toxicology – chromosomal aberration	Y	Y	Y	Y	N
Reproductive	Y	Y	Y	Y	N
Developmental	Y	Y	Y	Y	N

[a] U = undetermined

[b] -- means not applicable

[c] New data is italicized and bolded.